- Lagrange interpolation.
- Newton forward difference polynomials.
- Trapezoidal rule (revisited).
- Simpson's rule (revisited).
- Simpson's 3/8 rule.
- Integration error.

Lagrange Interpolation

Let us assume a set of numbers $x_0, \ldots, x_n$ and the corresponding function's ($f(x)$) values $f_0, \ldots, f_n$.

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There exist a unique polynomial $P_n\left(x\right)$ of degree n such that $P_n\left(x_i\right) = f_i$ for all $i = 0, \ldots, n$.

$$
\begin{aligned}
P_n(x) &= \sum_{i=0}^{n} C_i x^i \\
&= \sum_{i=0}^{n} a_i \prod_{i \neq j} (x - x_j)
\end{aligned}
$$

Lagrange Interpolation

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This polynomial is the Lagrange interpolation polynomial whose expression is given by :

$$\begin{aligned} P_n(x) &= \sum_{i=0}^{n} \frac{\prod_{j \neq i}(x - x_j)}{\prod_{j \neq i}(x_i - x_j)} f_i. \\ &= \prod_{i=0}^{n}(x - x_i) \sum_{i=0}^{n} \frac{f_i}{(x - x_i)\prod_{j \neq i}(x_i - x_j)}. \end{aligned}$$

Lagrange method is mostly a theoretical tool used for proving theorems. Not only it is not very efficient when a new point is added (which requires computing the polynomial again, from scratch), it is also numerically unstable.

Newton's divided differences Interpolation

If one writes the Lagrange interpolation polynomial slightly different basis functions, one obtains the Newton's interpolation formula given by:

$$\begin{aligned} P_n\left(x\right) = & \alpha_0 + \alpha_1\left(x - x_0\right) + \alpha_2\left(x - x_1\right)\left(x - x_0\right) + \ldots \\ & + \alpha_n\left(x - x_{n-1}\right)\ldots\left(x - x_1\right)\left(x - x_0\right) \end{aligned}$$

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For $i = 0$:

$$f_0 = P_n\left(x_0\right) = \alpha_0$$

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$$P_n(x) = \alpha_0 + \alpha_1 (x - x_0) + \alpha_2 (x - x_1)(x - x_0) + \dots \\ + \alpha_n (x - x_{n-1}) \dots (x - x_1)(x - x_0)$$

For $i = 0$:

$$f_0 = P_n(x_0) = \alpha_0$$

For $i = 1$:

$$f_1 = P_n(x_1) = \alpha_0 + \alpha_1(x_1 - x_0)$$
$$\alpha_1 = \frac{f_1 - f_0}{x_1 - x_0}$$

For $i = 2$:

$$f_2 = P_n(x_2) = \alpha_0 + \alpha_1(x_2 - x_0) + \alpha_2(x_2 - x_1)(x_2 - x_0)$$

$$\alpha_2 = \frac{(f_2 - f_1)/(x_2 - x_1) - (f_1 - f_0)/(x_1 - x_0)}{x_2 - x_0}$$

Similarly we can find $\alpha_3 \ldots\ldots \alpha_{n-1}$.

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Similarly we can find $\alpha_3.....\alpha_{n-1}$.
To express $\alpha_i, i = 0......n-1$ in a compact manner let us first define the following notation called divided differences:

$$f[x_k] = f_k$$

$$f[x_k, x_{k+1}] = \frac{f[x_{k+1}] - f[x_k]}{x_{k+1} - x_k}$$

$$f[x_k, x_{k+1}, x_{k+2}] = \frac{f[x_{k+1}, x_{k+2}] - f[x_k, x_{k+1}]}{x_{k+2} - x_k}$$

$$f[x_k, x_{k+1}, \ldots, x_i, x_{i+1}] = \frac{f[x_{k+1}, \ldots, x_{i+1}] - f[x_k, \ldots, x_i]}{x_{i+1} - x_k}$$

Newton's divided differences Interpolation

With this notation:

$$\alpha_0 = f[x_0]$$
$$\alpha_1 = f[x_0, x_1]$$
$$\alpha_2 = f[x_0, x_1, x_2]$$
$$\alpha_n = f[x_0, x_1, \dots, x_n]$$

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Now the polynomial can be rewritten as:

$$P_n(x) = \sum_{k=0}^{n} f[x_0, \ldots, x_k] \prod_{i=0}^{k-1} (x - x_i)$$

This is called as Newton's Divided Difference interpolation polynomial.

Sometimes in practice the data points x_i are equally spaced points:

$$x_i = x_0 + i \cdot h, \quad i = 0, 1, 2, \ldots, n$$

where x_0 is the starting point and h is the step size.

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These simple differences can be forward differences (Δf_i) or backward differences (∇f_i). We will first look at forward differences and the interpolation polynomial based on forward differences.

Newton's divided differences Interpolation

The first order forward difference Δf_i is defined as

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Newton's divided differences Interpolation

The first order forward difference Δf_i is defined as

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The second order forward difference $\Delta^2 f_i$ is defined as

$$\Delta^2 f_i = \Delta f_{i+1} - \Delta f_i$$

The k^{th} order forward difference $\Delta^k f_i$ is defined as

$$\Delta^k f_i = \Delta^{k-1} f_{i+1} - \Delta^{k-1} f_i$$

Then the first divided difference $f[x_0, x_1]$,

$$f[x_0, x_1] = \frac{f_1 - f_0}{h} = \frac{\Delta f_0}{h}$$

$\therefore \Delta f_0 = hf[x_0, x_1]$

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By the definition of second order forward difference $\Delta^2 f_0$, we get

$$\begin{aligned}
\Delta^2 f_0 &= \Delta f_1 - \Delta f_0 \\
&= h\{f[x_1, x_2] - f[x_0, x_1]\} \\
&= h * 2h\{(f[x_1, x_2] - f[x_0, x_1])/(x_2 - x_0)\} \\
&= 2h^2 f[x_0, x_1, x_2]
\end{aligned}$$

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In general,

$$\Delta^k f_i = k!h^k f[x_i, x_{i+1}, x_{i+2} ... x_{i+k}]$$

The Newton forward difference interpolation polynomial may be written as follows:

$$P_n(x) = \sum_{k=0}^{n} \frac{\Delta^k f_0}{k! h^k} \prod_{i=0}^{k-1} (x - x_i)$$

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We can rewrite the above in a simpler way:

$$x = x_0 + sh, \; p_n(s) = P_n(x)$$
$$x_k = x_0 + kh$$
$$x - x_k = (s - k)h$$

Then

$$\begin{aligned} p_n(s) &= \sum_{k=0}^{n} \frac{\Delta^k f_0}{k!h^k} \prod_{i=0}^{k-1} (s-i)h \\ &= \sum_{k=0}^{n} \frac{\Delta^k f_0}{k!h^k} \quad [s(s-1).......(s-k+1)]h^k \\ &= \sum_{k=0}^{n} \binom{s}{k} \Delta^k f_0 \end{aligned}$$

Error in interpolation

When interpolating a given function f by a polynomial of degree n at the nodes $x_0, \ldots, x_n$ we get the error

$$f(x) - P_n(x) = f[x_0, \ldots, x_n, x] \prod_{i=0}^{n} (x - x_i)$$

If f is $n+1$ times continuously differentiable then for each x in the interval there exists ξ in that interval such that

$$f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i)$$

The Trapezoidal Rule (revisited)

A first degree polynomial for a single interval (two points):

$$\Delta I = h \int_0^1 (f_0 + s\Delta f_0) ds = h \left[s f_0 + \frac{s^2}{2} \Delta f_0 \right]_0^1$$

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$$\Delta I = h(f_0 + \frac{1}{2}\Delta f_0) = \frac{h}{2}(f_0 + f_1)$$

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Applying over all intervals:

$$I = \sum_{i=0}^{n-1} \Delta I_i = \sum_{i=0}^{n-1} \frac{h}{2}(f_i + f_{i+1}) = \frac{h}{2}(f_0 + 2f_1 + \ldots + 2f_{n-1} + f_n)$$

The Trapezoidal Rule (revisited)

The error estimation can be done by integrating the error term. For a single interval:

$$E = h\int_0^1 \frac{s(s-1)}{2}h^2 f''(\xi)ds = -\frac{1}{12}h^3 f''(\xi) \sim \mathcal{O}(h^3)$$

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Total error:

$$E_T = \sum_{i=0}^{n-1} E_i = -\frac{1}{12}(x_n - x_0) h^2 f''(\xi) \sim \mathcal{O}(h^2)$$

where $x_0 \leq \xi \leq x_n$.

The Simpson's Rule (revisited)

A second degree polynomial for two intervals (three points):

$$\Delta I = h\int_0^2 (f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0)ds$$

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$$\Delta I = h \int_0^2 (f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0)ds$$

$$\Delta I = \frac{h}{3}(f_0 + 4f_1 + f_2)$$

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Applying over all intervals:

$$I = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots + 4f_{n-1} + f_n)$$

The Simpson's Rule (revisited)

The error estimation can be done by integrating the error term. For an interval:

$$E = h \int_0^2 \frac{s(s-1)(s-2)}{6} h^3 f'''(\xi) ds = 0$$

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$$E = h\int_0^2 \frac{s(s-1)(s-2)(s-3)}{24}h^4 f''''(\xi)ds = -\frac{1}{90}h^5 f''''(\xi)$$

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Total error:

$$E_T \sim \mathcal{O}(h^4)$$

The Simpson's 3/8 Rule

A third degree polynomial for three intervals (four points):

$$\Delta I = h \int_0^3 (f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{6}\Delta^3 f_0) ds$$

The Simpson's 3/8 Rule

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$$\Delta I = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

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$$\Delta I = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

Applying over all intervals:

$$I = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + 2f_3 + \ldots + 3f_{n-1} + f_n)$$

The Simpson's 3/8 Rule

The error estimation can be done by integrating the error term. For an interval:

$$E = h\int_0^3 \frac{s(s-1)(s-2)(s-3)}{24} h^4 f''''(\xi)ds = -\frac{3}{80}h^5 f''''(\xi)$$

The Simpson's 3/8 Rule

The error estimation can be done by integrating the error term. For an interval:

$$E = h\int_0^3 \frac{s(s-1)(s-2)(s-3)}{24} h^4 f''''(\xi) ds = -\frac{3}{80} h^5 f''''(\xi)$$

Total error:

$$E_T \sim \mathcal{O}(h^4)$$

Same order as Simpson's 1/3 rule!

Quadrature isa weighted sum of finite number of sample values of the intergrand.

$$\int_a^b f(x)dx = \sum_{i=1}^{n} f(x_i)w_i$$

name	degree	Weights
Trapezoid	1	(h/2, h/2)
Simpson's	2	(h/3, 4h/3, h/3)
3/8	3	(3h/8, 9h/8, 9h/8, 3h/8)
Milne	4	(14h/45, 64h/45, 24h/45, 64h/45, 14h/45)

Integration error

- The best numerical evaluation of an integral can be done with relatively small number of sub-intervals ($n \sim 1000 - 10000$).
- It is possible to get errors close to machine precision with Simpson's rule and other higher order methods.